Mass Spectrometers

Mass Spectrometers: A Short Explanation for the Absolute Novice

What does a mass spectrometer do?

A mass spectrometer produces charged particles (ions) from the chemical substances that are to be analyzed. The mass spectrometer then uses electric and magnetic fields to measure the mass ("weight") of the charged particles.

What are mass spectrometers used for?

Mass spectrometers are used for all kinds of chemical analyses, ranging from environmental analysis to the analysis of petroleum products, trace metals and biological materials (including the products of genetic engineering).

What does the mass tell us?

Let us use water (H_2O) as an example. A water molecule consists of two hydrogens (H) and one oxygen (O). The total mass of a water molecule is the sum of the mass of two hydrogens (approximately 1 atomic mass unit per hydrogen) and one oxygen (approximately 16 atomic mass units per oxygen):

H: 1 u (atomic mass units)
+ H: 1 u
+ O: 16 u

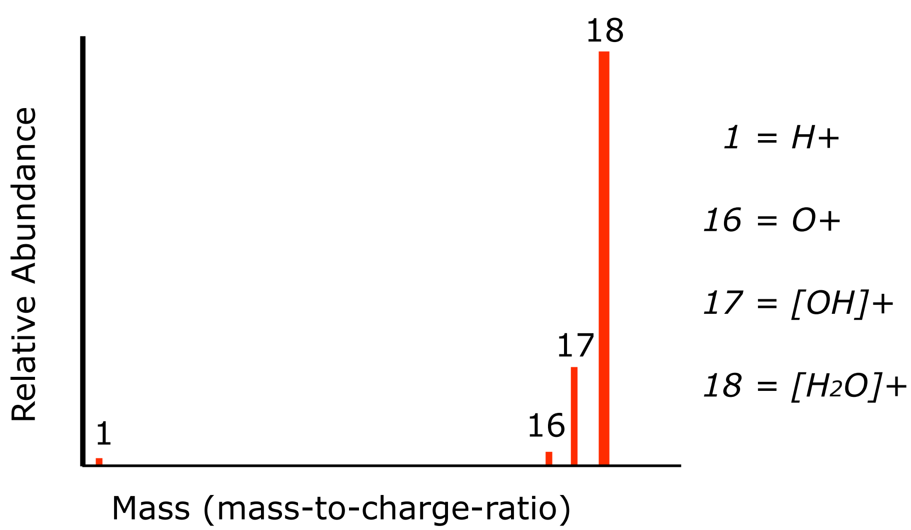
= H2O: 18 u

Let us then suppose that we put some water vapor into the mass spectrometer. A very small amount of water is all that is needed. The water is introduced into a vacuum chamber (the "ion source") of the mass spectrometer. If we shoot a beam of electrons through the water vapor, some of the electrons will hit water molecules and knock off an electron. If we lose a (negatively charged) electron from the (neutral) water molecule, the water will be left with a net positive charge. In other words, we have produced charged particles, or "ions" from the water:

H2O + 1 (fast) electron --> $[H2O]^+$ + 2 electrons

Some of the collisions between the water molecules and the electrons will be so hard that the water molecules will be broken into smaller pieces, or "fragments ". For water, the only possible fragments will be $[OH]^+$, O^+, and H^+.

The mass spectrum of water will show peaks that can be assigned to masses of 1, 16, 17, and 18, or:



Mass Spectrum of Water

Only certain combinations of elements can produce ions that have these masses. For example, the ammonium ion $[NH4]^+$ also has an approximate mass of 18 atomic mass units, but there would be peaks at mass 14 and 15 in the mass spectrum of ammonia corresponding to a N^+ and $[NH]^+$ (nitrogen is atomic mass 14).

A trained mass spectrometrist can interpret the masses and relative abundances of the ions in a mass spectrum and determine the structure and elemental composition of the molecule. It has been said that "*a mass spectrometrist is someone who figures out what something is by smashing it with a hammer and looking at the pieces*". Computer programs, such as those that search libraries of mass spectra for the best match, can also be used to interpret a mass spectrum.

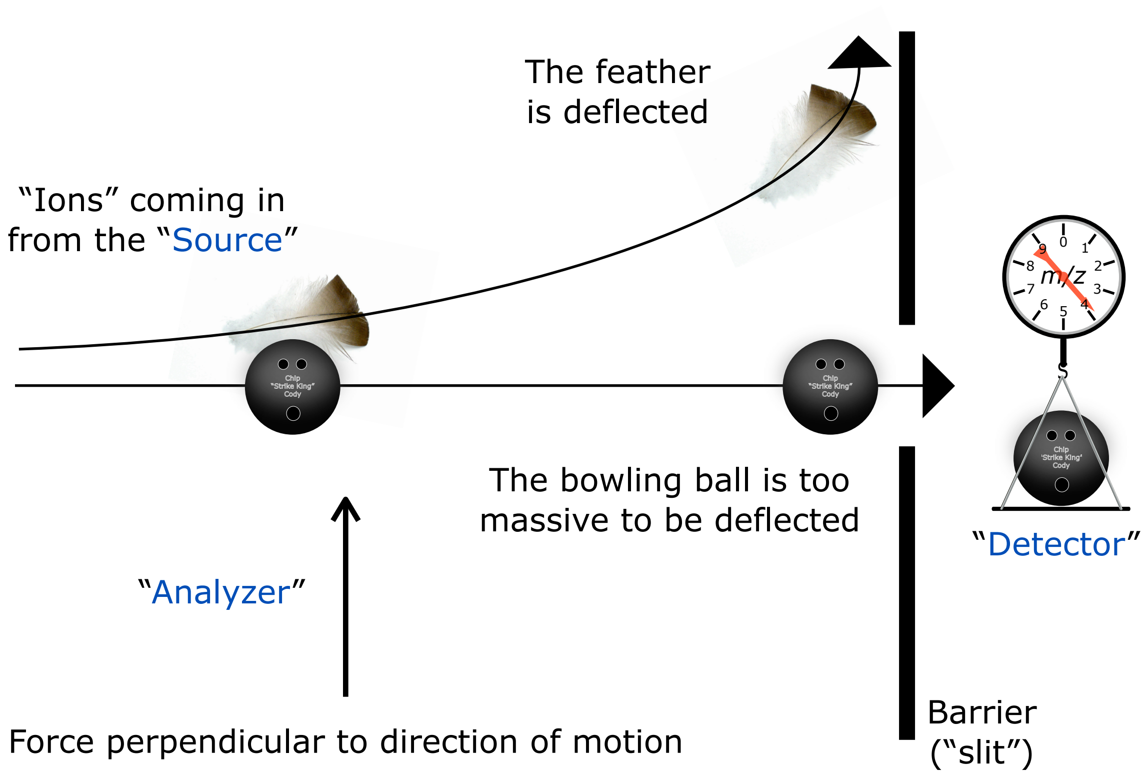
Mass spectra can provide other information as well. For example, a high-resolution mass spectrometer (such as those manufactured by JEOL) can determine the mass of an ion very precisely. If we knew that the mass of our hypothetical ion at mass 18 was actually mass 18.010, we could easily distinguish it from an ammonium ion, which would have an exact mass of 18.035 (we would not have to look for mass 14 and 15...). Given an accurate mass, and an estimated error tolerance, a computer can easily calculate the elemental composition of the molecule.

How does a mass spectrometer work?

There are many different kinds of mass spectrometers, but all use magnetic and/or electric fields to exert forces on the charged particles produced from the chemicals to be analyzed. A basic mass spectrometer consists of three parts:

1. A **source** in which ions are produced from the chemical substances to be analyzed.
2. An **analyzer** in which ions are separated according to mass.
3. A **detector** which produces a signal from the separated ions.

A magnetic field (in a "magnetic sector analyzer") separates ions according to their momentum (the product of their mass times their velocity). To understand how the force exerted by a magnetic field can be used to separate ions according to their mass, let us imagine that we have a bowling ball and a feather moving by us (both move at the same velocity). If we blow on the two objects in a direction perpendicular to the path of the objects, the feather will be deflected away from its path because it has a smaller mass (momentum), but the bowling ball, with its larger mass (momentum) will continue to move in its original path.



Separation of Masses in a "Mass Spectrometer"

JEOL produces "double-focusing mass spectrometers" that have analyzers with both an electric sector and a magnetic sector.

> The electric sector separates ions according to their *kinetic energy* ($\frac{1}{2}mv^2$)

The magnetic sector separates the ions according to their *momentum* (mv)

The combination of the two sectors provides very high resolution, or separating ability. JEOL also produces “time-of-flight mass spectrometers”. See “Summary of the Characteristics of Different Mass Analyzers” for more information on this analyzer type.

Information in a Mass Spectrum:

Exact mass: Elemental composition

Fragmentation pattern: Structure & "fingerprint "

Isotope abundances: Presence & number of certain elements

"Tricks" and Techniques

Forming Charged Particles (Ions):

- Electron impact (EI)
- Chemical Ionization (CI)
- Fast atom bombardment (FAB)
- Field desorption (FD)
- Electrospray ionization (ESI)
- Laser desorption (LD)

Analyzing Mixtures: Combine mass spectrometer with a:

- Gas chromatograph (GC/MS)
- Liquid chromatograph (LC/MS)

Interpreting the Results:

- Library search
- Exact masses give possible elemental compositions
- Interpretive computer programs
- Chemist interprets the spectrum